Spectroscopy of heavy nuclei by configuration mixing of symmetry restored mean-field states: Shape coexistence in neutron-deficient Pb isotopes

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Abstract

We study shape coexistence and low-energy excitation spectra in neutron-deficient Pb isotopes using configuration mixing of angular-momentum and particle-number projected self-consistent mean-field states. The same Skyrme interaction SLy6 is used everywhere in connection with a density-dependent zero-range pairing force.

Methods well suited to describe microscopically medium and heavy nuclei are based on effective energy functionals and self-consistent mean-field models [1]. They are successful for the description of many nuclear properties, but do not give direct access to low-energy spectroscopy, which in many cases requires to include correlations beyond the mean field approach. Broken symmetries can be restored by projection. Particle-number projection removes spurious contributions coming from states with different particle numbers, which are an artifact of the usual BCS approach. Angular momentum projection restores rotational symmetry and generates wave functions in the laboratory frame which provide transition probabilities and spectroscopic moments without further approximations. Finally, the variational configuration mixing with respect to a collective coordinate by means of the Generator-Coordinate Method (GCM) allows for an improved calculation of nuclear ground-state properties, as it removes the contributions from spurious collective vibrations that are inevitably mixed to the mean-field states. Besides that, a GCM calculation provides the excitation spectrum corresponding to given collective coordinates.

A model that combines these extensions of the mean-field approach offers a powerful tool: from a numerical point-of-view it is still simple enough to be applied to all up to superheavy nuclei, using the full model space of single-particle states with realistic asymptotics and the proper coupling to the continuum. Correlations corresponding to collective modes can be incorporated step by step into the modeling which helps to identify the relevant degrees of freedom.

The method has the advantage that its results can be interpreted within the intuitive picture of intrinsic shapes and shells of single-particle states that is offered by the framework of mean-field models.

We present here an application of a method based on these principles to neutron-deficient Pb isotopes around ^{186}Pb. The ground state of Pb isotopes is known to be spherical down to ^{182}Pb. However, weakening of the $Z = 82$ shell manifests itself by the appearance of low-lying 0^+ states [2]. At least one low-lying excited 0^+ state has been observed in all even-even Pb isotopes between ^{182}Pb and ^{194}Pb at excitation energies below 1 MeV, the most extreme cases being ^{186}Pb [3] with two excited 0^+ states below 700 keV.

The Method

The starting point of our method is a set of HF+BCS wave functions $|q\rangle$ generated by self-consistent mean-field calculations with a constraint on a collective coordinate q. Such mean-field states break several symmetries of the exact many-body states. Wave functions with good angular momentum and particle numbers are obtained by restoration of rotational and particle-number symmetry on $|q\rangle$:

$$|JMq\rangle = \frac{1}{\mathcal{N}} \sum_K g_K^J \hat{P}_{MK}^J \hat{P}_Z \hat{P}_N |q\rangle, \tag{1}$$

where $\mathcal{N}$ is a normalization factor. $\hat{P}_{MK}^J$, $\hat{P}_N$, $\hat{P}_Z$ are projectors onto angular momentum J with projection M along the laboratory z-axis, neutron number N and proton number Z respectively. We impose here axial symmetry and time reversal invariance on the intrinsic states $|q\rangle$. Therefore, K can only be 0 and we shall omit the coefficient $g_K^J = \delta_{K0}$. A variational configuration mixing on the collective variable q is then performed for each J

$$|JMk\rangle = \sum_q f_k^{JM}(q) |JMq\rangle. \tag{2}$$

The weight functions $f_k^{JM}(q)$ are determined by requiring that the expectation value of the energy

$$E_k^{JM} = \frac{\langle JMk|\hat{H}|JMk\rangle}{\langle JMk|JMk\rangle}, \tag{3}$$

is stationary with respect to an arbitrary variation $\delta f_k^{JM}(q)$. This prescription leads to the discretized Hill-Wheeler equation. Collective wave functions in the basis of the intrinsic states are then obtained from the set of weight functions

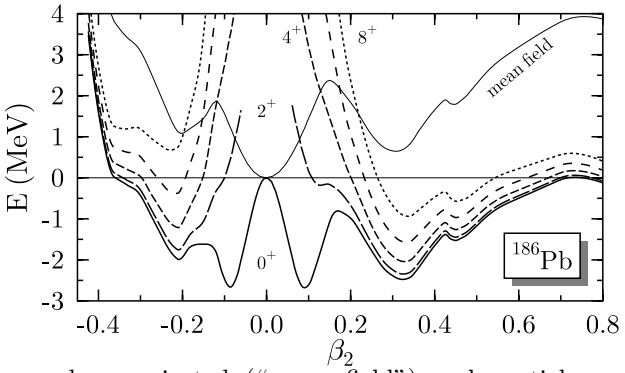

Figure 1: Particle-number projected ("mean field") and particle-number and angular-momentum projected potential energy curves up to $J = 10$ for ^{186}Pb as a function of the mass quadrupole deformation β_2.

$f_k^{JM}(q)$ by a basis transformation [4]. In $|JMk\rangle$, the weight of each mean-field state $|q\rangle$ is given by:

$$g_k^{JM}(q) = \langle JMk|q\rangle \quad . \tag{4}$$

Since the collective states $|JMk\rangle$ have good angular momentum, quadrupole moments and transition probabilities can be directly determined in the laboratory frame of reference without further approximations. For further details on the evaluation of overlaps and matrix elements see [5].

The same effective interaction is used to generate the mean-field wave functions and for the configuration mixing calculation. We have chosen the Skyrme interaction SLy6 in the mean-field channel [6] and a density-dependent zero-range force as defined in [7] in the pairing channel.

An illustrative example: ^{186}Pb

We discuss ^{186}Pb as an example for the results that can be obtained with the method; see ref. [8] for more details. On figure 1 is plotted the deformation energy of ^{186}Pb before and after projection on angular momentum. All curves are drawn versus the intrinsic axial quadrupole moment of the unprojected mean-field states. As projected $J = 0$ states are spherical, this "quadrupole moment" is only a convenient way to label the projected states. The curve labeled "mean-field" plots the deformation energy after particle-number projection only. It exhibits a spherical global minimum as well as local minima at prolate and oblate deformations. While the deformation energy of the prolate minimum fortuitously reproduces the experimental value of 0.650 MeV for the prolate 0^+ state, the 1.1 MeV deformation energy of the oblate minimum overestimates the experimental value of 0.532 MeV for the oblate 0^+ state.

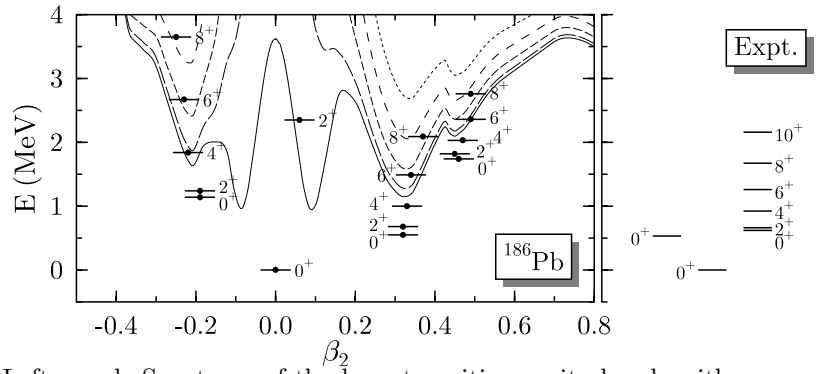

Figure 2: Left panel: Spectrum of the lowest positive parity bands with even angular momentum and $K = 0$, as a function of the deformation (see text). The angular momentum projected energy curves are shown for comparison. The energy reference is that of the calculated 0^+_1 ground state. Right panel: Available experimental excitation energies [3, 9]. From the left to the right the spectrum shows oblate, spherical and prolate states.

The energy curves obtained after angular momentum projection are also shown on figure 1. The spherical mean-field state is rotationally invariant and therefore contributes to $J = 0$ only. Two minima appear at small deformations around $\beta_2 = \pm 0.1$. They do not correspond to two different states, but to the correlated spherical state (see below).

The excitation energies E^{JM}_k of the collective states $|JMk\rangle$ obtained from the configuration mixing calculation are shown in figure 2. Each of these states is represented by a bar drawn at the average intrinsic deformation of the mean-field states it is built from. The excitation spectrum is divided into bands corresponding to different deformations. Configuration mixing lowers the energy of the lowest collective states with respect to the projected energy curves; the energy gain is the largest for the ground state. The available data are plotted on the right panel of figure 2. The calculated energy of the prolate 0^+ state is very close to the experimental energy contrary to the excitation

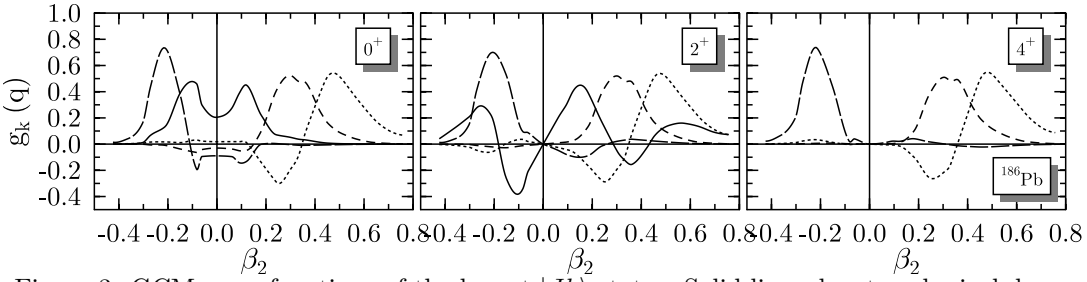

Figure 3: GCM wave functions of the lowest $|Jk\rangle$ states. Solid lines denote spherical, long-dashed lines oblate, dashed lines prolate, dotted lines the β band in the prolate well.

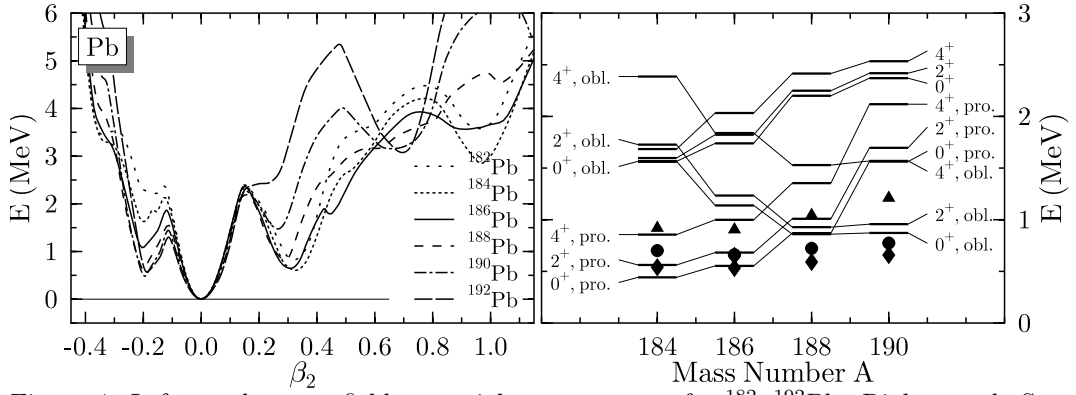

Figure 4: Left panel: mean-field potential energy curves for $^{182-192}$Pb. Right panel: Systematics of low-lying states. The two lowest calculated 0^+ and 2^+ states in ^{188}Pb are nearly degenerate. Filled diamonds, circles, and triangles denote the lowest known excited 0^+, 2^+, and 4^+ states respectively. Data taken from [2].

energy of the oblate 0^+ state which is largely overestimated.

The corresponding collective wave functions $g_k^{JM}(q)$ are plotted in figure 3. The ground state wave-function is spread in a similar way on both oblate and prolate sides with a zero average quadrupole deformation. The wave functions of the first two excited 0^+ states are strongly peaked at either prolate or oblate deformations, with their tails extending into the spherical well. Starting with $J = 4$, states are localized and are predominantly either prolate or oblate. The shapes of the 0_4^+, 2_3^+, and 4_3^+ wave functions suggests their interpretation as a rotational band built onto a β vibration within the prolate well.

Calculated transition probabilities for $J > 2$ states confirm the separation of the excited states into rotational bands with very small $B(E2)$ transitions between bands, while the large branching of $E2$ strength for the in and out of bands $2^+ \rightarrow 0^+$ transitions reflects that the low-lying 0^+ states are mixed.

Systematics

The systematics of the potential energy surfaces for the Pb isotopes with $A = 182 - 192$ is shown in the left panel of figure 4. It can be clearly seen that the oblate minimum is pushed up in energy and disappears below $A = 184$, while a prolate minimum develops below $A = 192$. Various superdeformed structures can be seen at large deformation. The pattern is reflected in the systematics of the excitation energies of the 0^+, 2^+ and 4^+ states in the three lowest rotational bands obtained from the configuration mixing for $A = 184 - 190$, see the right panel of figure 4. Calculated oblate and prolate bands cross for ^{188}Pb, at slightly larger neutron number than suggested by experiment [2].

For the three heavier isotopes, the third band has a similar structure as the one obtained for ^{186}Pb, while for ^{184}Pb it corresponds to the superdeformed minimum around $\beta_2 = 1.0$.

Conclusions

Systematic calculations of spectroscopic properties of very heavy nuclei based on self-consistent mean-field methods have become feasible, as has been shown on the example of low-lying excited states in neutron-deficient Pb isotopes. Our results strongly support the interpretation of the Pb spectra as a manifestation of shape coexistence. There remains, however, a significant overestimation of the oblate band's excitation energy in some of the nuclei, which can be due to the one or the other ingredient of the model: (1) the effective mean-field interaction (as surface tension, spin-orbit splitting, etc), (2) the strength and the form factor of the pairing interaction, (3) missing collective modes in the configuration mixing, or (4) a necessary generalization of the density dependence of the effective interaction for calculations beyond mean field as suggested in ref. [10]. The effective interactions clearly deserve future reexamination. Various generalizations of the model are underway.

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